

APPENDIX C. USE OF CFT MODEL DATA FOR CALIBRATION

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1 Description of CFT Model Output

This appendix describes how the contaminant fate and transport (CFT) model output was summarized for use in the bioaccumulation model. The data from the CFT model used to calibrate the bioaccumulation model were those used in the April 2015 draft feasibility study (Integral [in prep]). The following provides details regarding the CFT model output that was used to calibrate the bioaccumulation model:

- ◆ Data included monthly average values for three years of model output (October 2010 to September 2013).
- ◆ Values were provided for a total of 26 spatial areas (13 spatial segments for both river-wide and mudflat-only areas). The three spatial scales that were directly used in model calibration were site wide, river mile (RM) 4 to Dundee Dam, and RM 7 to Dundee Dam. Both river-wide (i.e., bank-to-bank) and mudflat-only values were used based on the selected modeling area for fish (Section 3.2.3 of the main document).
- ◆ Model runs were provided for two chemicals: 2,3,7,8-tetrachlorodibenzo-*p*-dioxin (TCDD) and tetrachlorobiphenyl (tetraCB)
- ◆ CFT model output included nine parameters (including five that were chemical specific) that were used as inputs for the bioaccumulation model. These included chemical concentrations, water temperature, and organic carbon content (Table 1).

Table 1 provides a summary of the nine parameters derived from the CFT model output that were used to calibrate the bioaccumulation model.

Table 1. Bioaccumulation model parameters derived from CFT model output

Parameter Name	Model Code	Units	Notes
Chemical-specific parameters:			
Chemical concentration in sediment	CST	ng/g dw	top 2 sediment layers; area-weighted average
Chemical concentration in porewater	CSD	ng/g	area-weighted average
Chemical concentration in bioavailable water	CWB	ng/g	volume-weighted average
Chemical concentration in water column particulates	CPART	ng/g dw	volume-weighted average
Chemical concentration in near-bottom ^a particulates	CPART_DET	ng/g dw	area-weighted average
Non-chemical-specific parameters:			
Mean water temperature	TW	°C	area-weighted average
OC content of sediment	OCSS	fraction	top 2-cm layer; area-weighted average
OC content of water column particulates	OCPART	fraction	volume-weighted average
OC content of near-bottom particulates	OCPART_DET	fraction	area-weighted average

^a A total of 10 layers are used to model the water column. Each layer consists of 10% of the water column depth in a given cell. Near-bottom particulates are the particulates in the bottom layer of the water column and are used to represent the chemical concentrations in detritus at the sediment-water column interface.

CFT – contaminant fate and transport
dw – dry weight

The following describes the averaging of the CFT model output for the various parameters:

- ◆ **Daily averages** – Averages for each day were provided for each parameter.
- ◆ **Spatial resolution** – The Lower Passaic River Study Area (LPRSA) CFT model is divided into cells (i.e., areas), each of which is modeled individually. Cells are averaged by area or volume (depending on the parameter, as noted in Table 1) to obtain values for larger areas (e.g., RM 4 to 17.4) evaluated in the bioaccumulation model.
- ◆ **Water column depth layers** – A total of 10 layers are used to model the water column. Each layer consists of 10% of the water column depth in a given cell.
- ◆ **Sediment bed depth layers** – As with the water column, the bedded sediment is modeled in layers. The depth of the top layer is variable, ranging from 0.5 to 2 cm. After the first layer, each subsequent layer has a depth of 1 cm. The bioaccumulation model uses the top two sediment bed depth layers.

Table 2 lists the CFT model parameters used to calculate the bioaccumulation model parameters presented in Table 1. Table 3 presents the equations used to convert the CFT model parameters to those needed for the bioaccumulation model.

Table 2. Definition of CFT model parameters

Parameter	Parameter Description
TW	water temperature (°C)
C _{wc,diss,1-10}	depth-average dissolved concentration in water column
DOC _{wc}	dissolved organic carbon concentration in water column
K _{ow}	octanol-water partitioning coefficient
C _{wc,part,1-10}	depth-average concentration in particulates in water column
TSS _{wc,1-10}	depth-average concentration of suspended solids in water column
POC _{wc,1-10}	depth-average particulate organic carbon concentration in water column
POC _{wc,10}	particulate organic carbon concentration in bottom layer of water column
C _{wc,part,10}	concentration in particulates in bottom layer of water column
TSS _{wc,10}	concentration of suspended solids in bottom layer of water column
C _{bed,diss,1-X}	depth-average dissolved concentration in sediment bed between layers 1 and X
Φ	porosity
TSS _{bed,1-X}	depth-average concentration of suspended solids in sediment bed between layers 1 and X
ρ _{water}	specific gravity of water (constant equal to 1 ^a)
C _{bed,part,1-X}	depth-average concentration in particulates in sediment bed between layers 1 and X
POC _{bed,1-X}	depth-average organic carbon concentration in particulates in sediment bed between layers 1 and X

^a Values for these constants are current CFT model output is from October 31, 2014 (with updates provided on January 14 and March 2, 2015). current as of February 18, 2015.

CFT – contaminant fate and transport
DOC – dissolved organic carbon
TSS – total suspended solids
POC – particulate organic carbon

Table 3. Equations used to calculate bioaccumulation model parameters from CFT model parameters

Bioaccumulation Model Parameter		Equation from CFT Parameters ^a
Model Code	Name	
Chemical specific parameters		
CST	Chemical concentration in sediment	= C _{bed,part,1-X} / TSS _{bed,1-X}
CSD	Chemical concentration in porewater	= C _{bed,diss,1-X} / ρ _{water}
CWB	Chemical concentration in bioavailable water	= C _{wc,diss,1-10} /(1 + K _{ow} x ADOC x DOC _{wc})
CPART	Chemical concentration in water column particulates	= C _{wc,part,1-10} / TSS _{wc,1-10}
CPART_DET	Chemical concentration in near-bottom particulates	= C _{wc,part,10} / TSS _{wc,10}
Non-chemical specific parameters		
TW	Mean water temperature	= TW
OCSS	OC content of sediment	= POC _{bed,1-X} / TSS _{bed,1-X}
OCPART	OC content of water column particulates	= POC _{wc,1-10} / TSS _{wc,1-10}
OCPART_DET	OC content of near-bottom particulates	= POC _{wc,10} / TSS _{wc,10}

^a The second term in the subscript designates the CFT model layer(s) (water column or sediment bed) included in the calculation.

ADOC – DOC proportionality constant (Arnot and Gobas 2004)

CFT – contaminant fate and transport

DOC – dissolved organic carbon

2 Summary of Data Used in Bioaccumulation Model Calibration

CFT model output was averaged over the calibration period (2011–2013) to develop exposure concentrations for the steady state model. The average values used in model calibration for each parameter are presented in Table 4 and 5 for chemical-specific parameters (for 2,3,7,8-TCDD and tetraCB, respectively) and Table 6 for non-chemical-specific parameters. Additionally, minimum and maximum values for each parameter are presented to indicate the range of values in the calibration dataset.

Table 4. Chemical-specific parameter values for 2,3,7,8-TCDD

Parameter Name	Unit	Spatial Segment	River-wide Parameter Values for 2,3,7,8-TCDD			Mudflats-only Parameter Values for 2,3,7,8-TCDD		
			Average	Minimum	Maximum	Average	Minimum	Maximum
Concentration in sediment solids	ng/g	site wide	0.46	0.36	0.78	0.37	0.18	0.75
		RM 4-DD	0.58	0.45	0.92	0.29	0.09	0.45
		RM 7-DD	0.64	0.46	0.98	0.29	0.08	0.46
Concentration in sediment porewater	ng/g	site wide	4.5E-06	3.4E-06	7.6E-06	2.9E-06	1.3E-06	5.7E-06
		RM 4-DD	6.5E-06	4.6E-06	1.0E-05	3.1E-06	9.7E-07	4.7E-06
		RM 7-DD	7.4E-06	5.2E-06	1.2E-05	3.1E-06	8.7E-07	4.8E-06
Bioavailable concentration in water	ng/g	site wide	2.5E-07	9.9E-08	6.0E-07	1.9E-07	9.5E-08	3.6E-07
		RM 4-DD	2.4E-07	6.7E-08	8.8E-07	7.0E-08	1.7E-08	4.0E-07
		RM 7-DD	1.9E-07	4.2E-08	8.8E-07	5.3E-08	1.1E-08	3.6E-07
Concentration in water column	ng/g	site wide	0.22	0.08	0.58	0.19	0.09	0.37
		RM 4-DD	0.25	0.05	0.90	0.09	0.01	0.43

particulates		RM 7-DD	0.22	0.03	0.99	0.07	0.006	0.40
Concentration in near-bottom particulates	ng/g	site wide	0.22	0.07	0.56	0.20	0.08	0.58
		RM 4-DD	0.26	0.04	0.90	0.10	0.01	0.46
		RM 7-DD	0.22	0.02	0.99	0.07	0.006	0.43

DD – Dundee Dam

RM – river mile

TCDD – tetrachlorodibenzo-*p*-dioxin

Table 5. Chemical-specific parameter values for tetraCB

Parameter Name	Unit	Spatial Segment	River-wide Parameter Values for TetraCB			Mudflats-only Parameter Values for TetraCB		
			Average	Minimum	Maximum	Average	Minimum	Maximum
Concentration in sediment solids	ng/g	site wide	232	193	359	232	164	368
		RM 4-DD	229	178	355	198	93	281
		RM 7-DD	217	156	306	190	81	277
Concentration in sediment porewater	ng/g	site wide	2.4E-03	1.4E-03	5.0E-03	2.4E-03	1.4E-03	4.5E-03
		RM 4-DD	3.0E-03	1.6E-03	6.1E-03	3.4E-03	1.8E-03	5.6E-03
		RM 7-DD	3.2E-03	1.7E-03	5.6E-03	3.4E-03	1.9E-03	5.7E-03
Bioavailable concentration in water	ng/g	site wide	6.0E-04	3.5E-04	1.1E-03	6.1E-04	4.1E-04	8.8E-04
		RM 4-DD	5.8E-04	2.7E-04	1.4E-03	5.7E-04	3.7E-04	1.0E-03
		RM 7-DD	5.4E-04	2.5E-04	1.4E-03	5.6E-04	3.7E-04	1.0E-03
Concentration in water column particulates	ng/g	site wide	216	127	373	228	146	313
		RM 4-DD	237	106	493	181	90	324
		RM 7-DD	234	93	504	169	80	294
Concentration in near-bottom particulates	ng/g	site wide	213	124	368	250	143	996
		RM 4-DD	240	100	502	186	84	339
		RM 7-DD	237	90	515	172	73	308

DD – Dundee Dam

RM – river mile

Table 6. Non-chemical-specific parameter values

Parameter Name	Spatial Segment	River-wide Parameter Values			Mudflat-only Parameter Values		
		Average	Minimum	Maximum	Average	Minimum	Maximum
Mean water temperature (°C)	site wide	13.3	1.3	25.2	13.3	1.4	25.2
	RM 4-DD	13.5	0.7	26.6	13.8	0.7	27.5
	RM 7-DD	13.6	0.7	26.8	13.8	0.7	27.6
Organic carbon content of sediment (fraction)	site wide	0.057	0.053	0.060	0.058	0.056	0.061
	RM 4-DD	0.046	0.043	0.050	0.037	0.036	0.039
	RM 7-DD	0.041	0.040	0.043	0.035	0.034	0.037
Organic carbon content of water column particulate (fraction)	site wide	0.13	0.07	0.15	0.12	0.08	0.15
	RM 4-DD	0.16	0.06	0.20	0.13	0.06	0.21
	RM 7-DD	0.18	0.06	0.24	0.13	0.05	0.21
Organic carbon content of near-bottom particulates	site wide	0.14	0.07	0.24	0.27	0.12	1.61
	RM 4-DD	0.18	0.07	0.23	0.28	0.10	0.43
	RM 7-DD	0.21	0.06	0.28	0.25	0.08	0.41

DD – Dundee Dam

RM – river mile

3 References

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